Supporting Information for

Simultaneous enhancements on the mechanical, thermal stability, and flame retardant properties of poly(1,4-butylene terephthalate) nanocomposites with a novel phosphorus-nitrogen-containing polyhedral oligomeric silsesquioxane

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Nanocomposite morphology

The dispersion and morphology of PBT/POSS and PBT/F-POSS were measured by transmission electron microscopy (TEM). The TEM images of the composites were obtained on a JEOL JEM-2100F with an accelerating voltage of 200 KV. The composite specimens were cut into ultrathin slices under cryogenic conditions with an ultramicrotome (Ultraacut-1, United Kingdom) equipped with a diamond knife. The cross-section morphology of PBT/POSS and PBT/F-POSS was characterized by TEM, as shown in Fig. S2. It is observed that the POSS nanoparticles are detected as spherical dark regions in Fig. S2 (a) owing to their high electron density.[1,2] The diameter of N-phenylaminopropyl-POSS is lower than 50 nm.[3,4] However, the size of the dark region observed in TEM image exceeds 100 nm, indicating slight agglomerations of POSS nanoparticles in the PBT matrix. POSS particles tend to form aggregates probably due to the strong hydrogen-bond interaction between H atoms in the amino groups and O atoms in the silica-like inorganic core. These POSS agglomerations or clusters in spherical form have been also found in the reported articles.[5,6-8] In order to compare with the background, the TEM image for PBT/F-POSS has been performed at the edge of the sectioned sample, which is shown in Fig. S2 (b). It is clearly seen that the dark area (the portion of the hybrid composite) is homogenous. There are also no large localized domains, indicating that the F-POSS particles are homogenously dispersed in PBT matrix at nanoscale. This phenomenon is in good agreement with the published articles.[9-11] In the functionalization process, the H atoms in amino groups of POSS is displaced by the P atoms in DPP-Cl, leading

to the disappearance of hydrogen-bond interaction between F-POSS particles. Therefore, the F-POSS particles are well distributed into PBT matrix at nanometer level during the melt processing.

Table S1. Tensile properties for each sample.

Sample	Tensile strength (MPa)	Elongation at break (%)
Neat PBT	49.5 ± 2.1	244 ± 10
PBT/POSS	52.7 ± 1.9	139 ± 18
PBT/F-POSS	55.6 ± 1.5	121 ± 15

Table S2. TGA data for each sample under nitrogen and air condition. (20 ^{o}C/min, 5-10 mg; Residue, obtained at 700 ^{o}C.)

Sample	N_2 atmosphere			Air atmosphere				
	$T_{-5\%}$ (^{o}C)	T_{max} (^{o}C)	Residue (wt%)	$T_{-5\%}$ (^{o}C)	T_{max1} (^{o}C)	T_{max2} (^{o}C)	Residue (wt%) at 600 ^{o}C	Residue (wt%) at 700 ^{o}C
Error	± 1	± 1	± 0.5	± 1	± 1	± 1	± 0.5	± 0.5
Neat PBT	367	408	2.7	373	406	545	0.4	0.4
PBT/POSS	380	414	4.9	376	412	581	3.1	1.0
PBT/F-POSS	382	416	6.7	376	418	598	5.0	2.9

Table S3. Cone calorimeter data for each sample at 50 kW/m^2. (t_{ign}: time to ignition; t_p: time to peak heat release rate; PHRR: peak heat release rate; THR: total heat release; PSPR: peak smoke production rate; TSP: total smoke production; PCOP: peak CO production; PCO_2P: peak CO_2 production.)

Sample	t_{ign} (s)	t_p (s)	PHRR (kW/m^2)	THR (MJ/m^2)	PSPR (m^2/s)	TSP (m^2/kg)	PCOP (g/s)	PCO_2P (g/s)	Residue (wt%)
Error	± 5	± 5	± 15	± 0.5	± 0.01	± 20	± 0.005	± 0.02	± 0.2
Neat PBT	52	150	1104	65.2	0.286	503	0.0423	1.179	3.5
PBT/POSS	67	180	1098	67.1	0.279	508	0.0416	1.165	5.9
PBT/F-POSS	60	210	556	62.7	0.155	493	0.0275	0.650	8.2

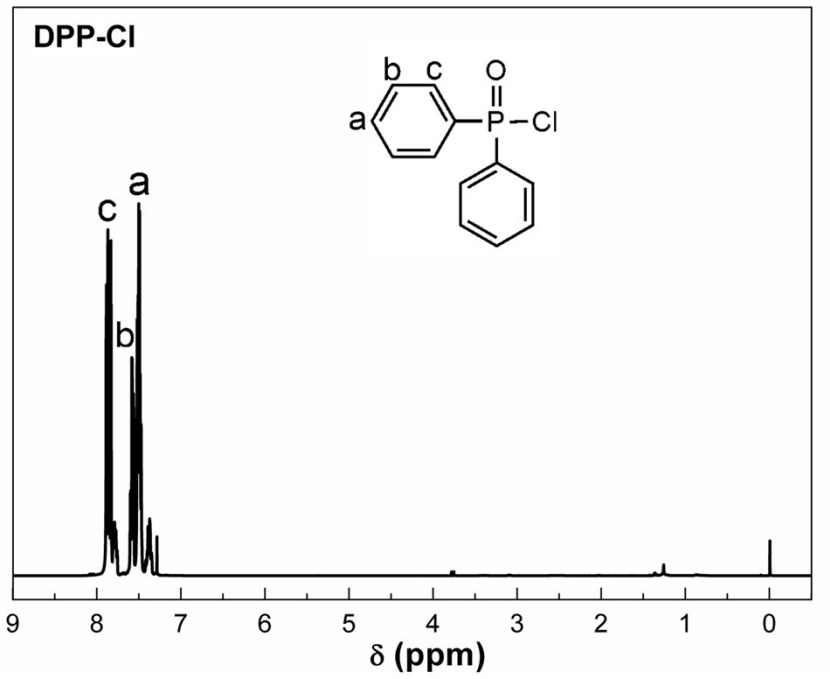

Fig. S1. ^{1}H NMR spectrum of DPP-Cl.

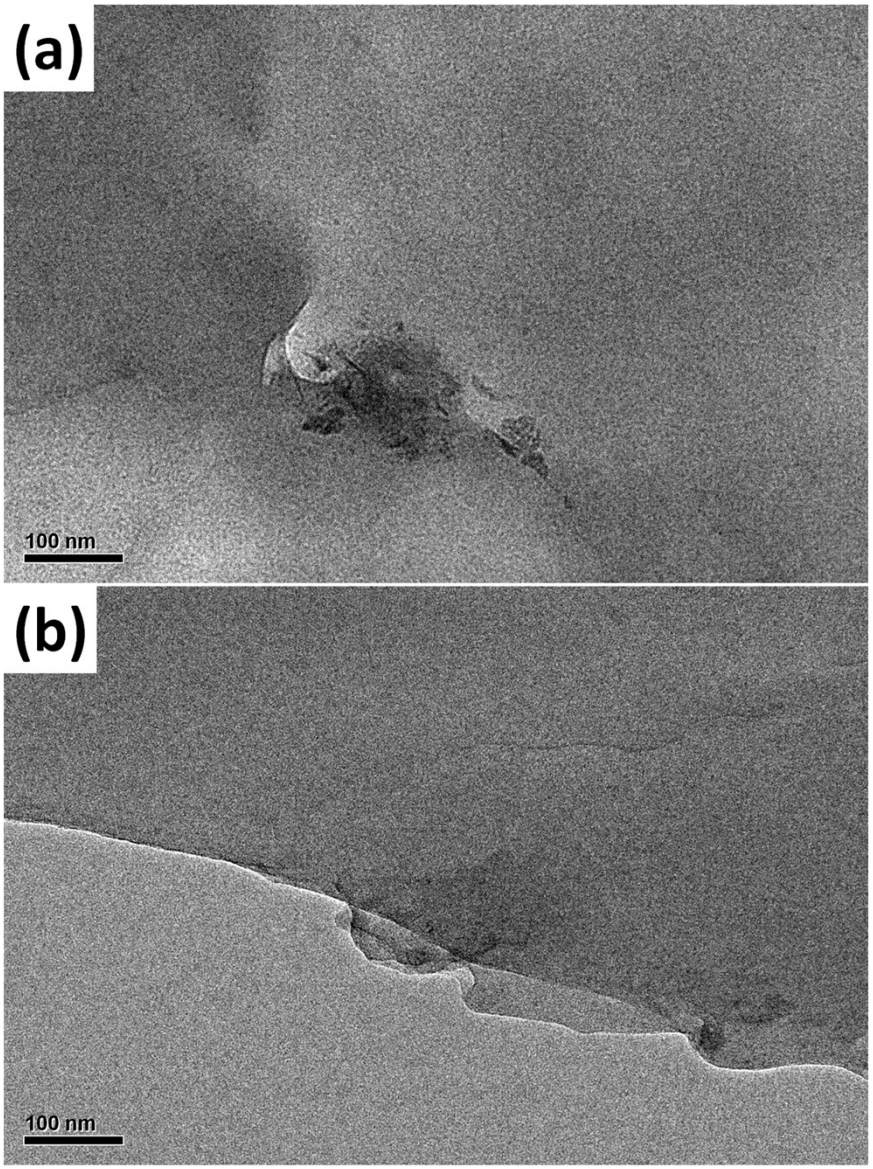

Fig. S2. TEM images of the nanocomposite fracture surfaces: (a) PBT/POSS; (b) PBT/F-POSS.

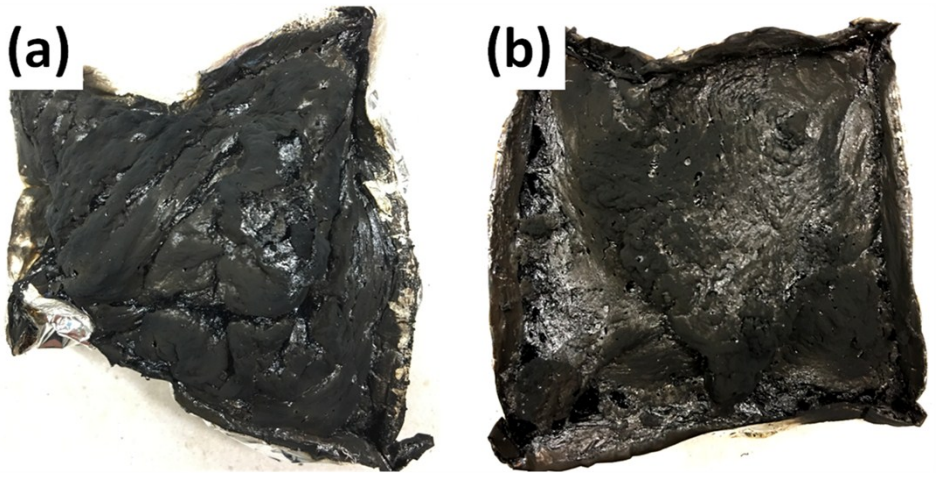

Fig. S3. Digital photographs of the residues after cone calorimeter testing: (a) PBT/POSS; (b) PBT/F-POSS.

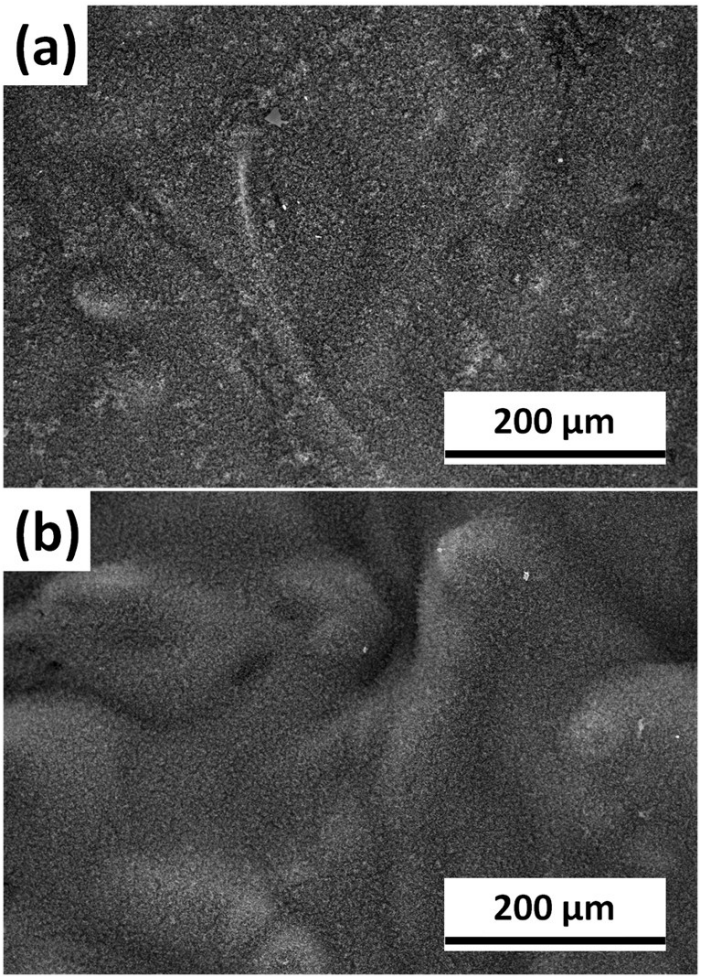

Fig. S4. SEM images of the outer residues after cone calorimeter testing in low magnification (×200): (a) PBT/POSS; (b) PBT/F-POSS.

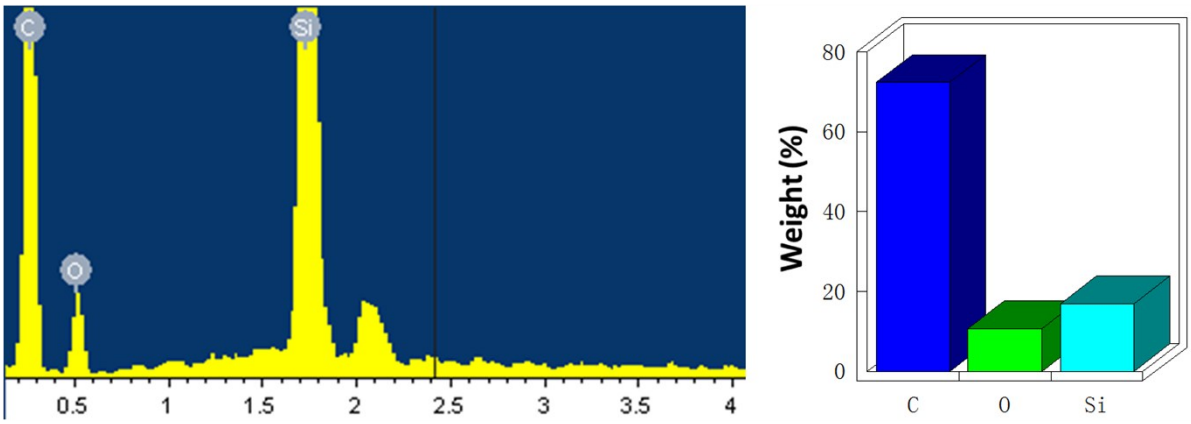

Fig. S5. EDX chemical compositions of outer residues for PBT/POSS.

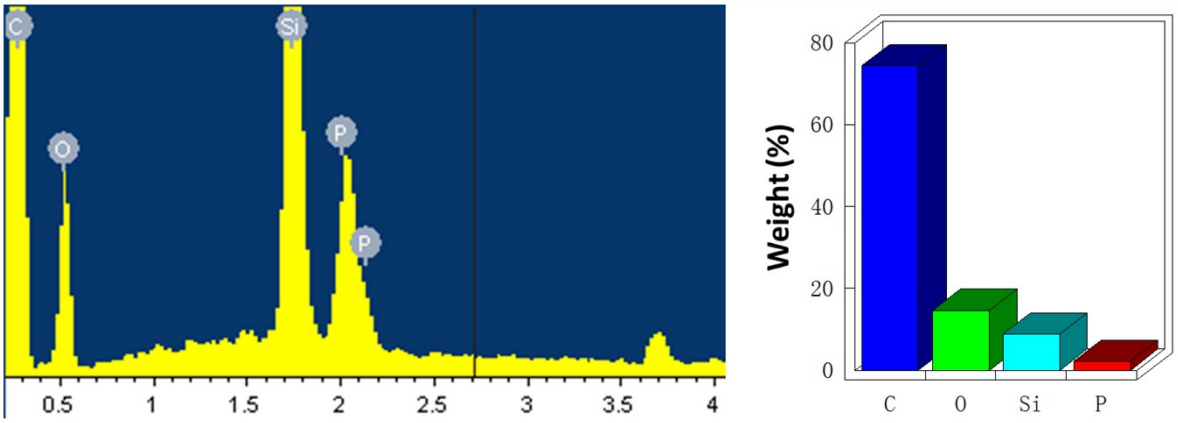

Fig. S6. EDX chemical compositions of outer residues for PBT/F-POSS.

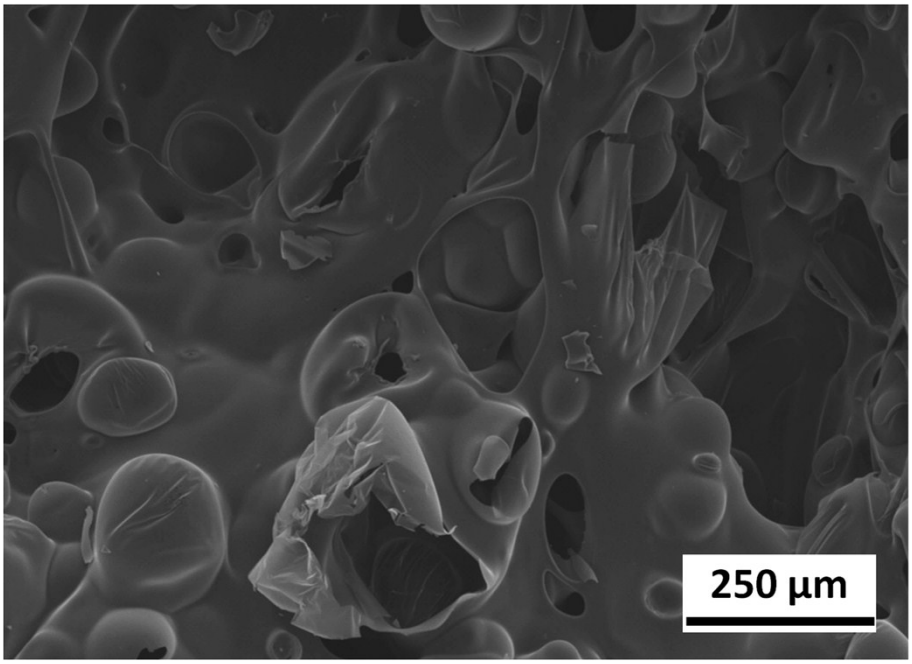

Fig. S7. SEM image of the inner residues for PBT/POSS after cone calorimeter testing in low magnification (×100).

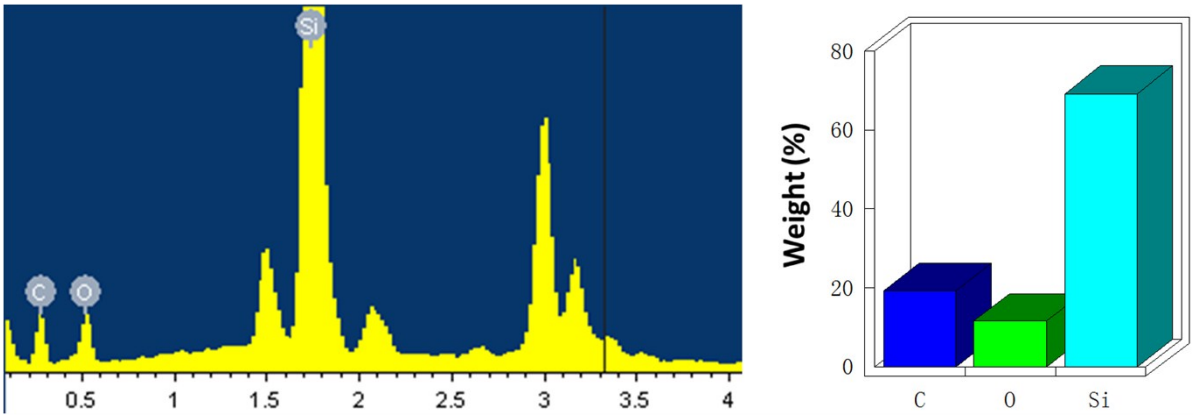

Fig. S8. EDX chemical compositions of inner residues for PBT/POSS.

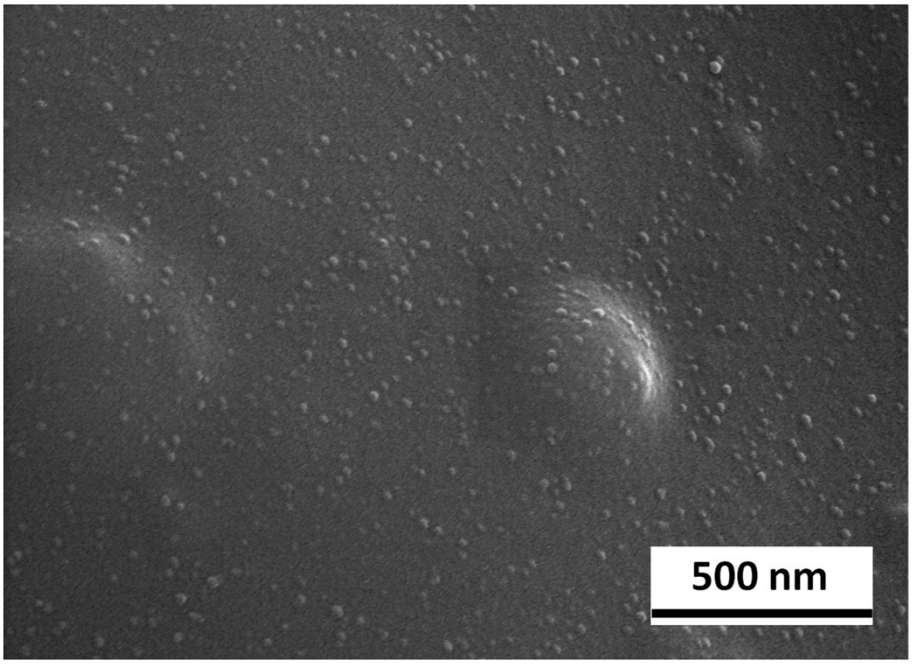

Fig. S9. SEM image of the inner residues for PBT/F-POSS after cone calorimeter testing in high magnification (×60000).

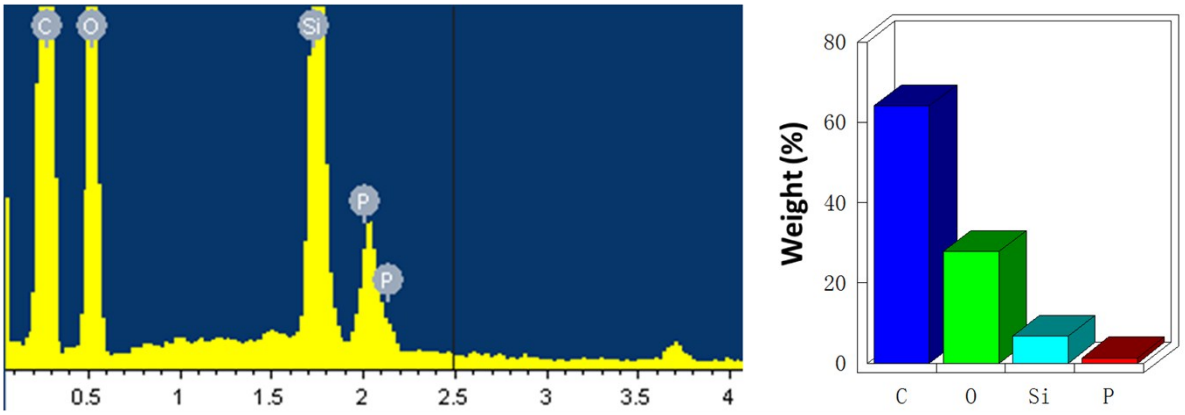

Fig. S10. EDX chemical compositions of inner residues for PBT/F-POSS.

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